

Morad Mustafa



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Department of Pharmacy
Al-Zaytoonah University of Jordan
P.O. Box: 130
Amman 11733, Jordan

Education

- 2009–2010: **Postdoctoral Training**
Department of Biochemistry and Molecular Biology, The University of Georgia, Athens, GA, USA.
Research Focus: Structure and function of lung cancer related protein kinases.
Mentor: Prof. Natarajan Kannan
- 2003–2008: **Ph.D., Computational Biophysical Chemistry**
Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA
Dissertation: Ion permeation through membrane channels: molecular dynamics simulations studies
Supervisors: Prof. Douglas J. Henderson
Prof. David D. Busath
- 1998–2001: **M.S. (First Class Honors), Physical Chemistry**
Department of Chemistry, Yarmouk University, Irbid, Jordan
Thesis: The role of cyclodextrin cavity size on the normal and twisted intramolecular charge transfer (TICT) fluorescence of *N,N*-disubstituted *p*-cyanoanilines in aqueous solutions
Supervisor: Prof. Khader Al-Hassan
- 1994–1998: **B.S. (First Class Honors), Chemistry**
Department of Chemistry, Yarmouk University, Irbid, Jordan

Teaching Interests

- ★ General Chemistry
- ★ Thermodynamic Chemistry
- ★ Kinetic Chemistry
- ★ Quantum Chemistry and Spectroscopy
- ★ Statistical Mechanics

Research Interests

- ★ Molecular Dynamics Simulations
- ★ Virtual Screening
- ★ Density Functional Theory Calculations

Professional Experience

- Feb, 2022 – Present: **Assistant Professor**, Department of Pharmacy, Al-Zaytoonah University of Jordan, Amman, Jordan.
- Jul, 2020 – Jan, 2022: **Assistant Professor** (Part Time), Department of Chemistry, The University of Jordan, Amman, Jordan.
- Apr, 2010 – Aug, 2019: **Assistant Professor**, Department of Chemistry, King Khalid University, Abha, Saudi Arabia.
- Apr, 2009 – Mar, 2010: **Postdoctoral Fellow**, Department of Biochemistry and Molecular Biology, The University of Georgia, Athens, GA, USA.
▶ Structure and function of lung cancer related protein kinases.
- 2003–2006: **Graduate Teaching Assistant**, Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA.
▶ Teaching assistant roles: conducting lectures, grading course assessment materials, and holding tutorials and office hours.
- 2002–2003: **Teaching Assistant**, Department of Chemistry, The University of Jordan, Amman, Jordan.
- 2001–2002: **Analyst**, Research and Development Department, Dar Al Dawa Veterinary and Agricultural Company, Amman, Jordan.
- 1998–2001: **Graduate Teaching Assistant**, Department of Chemistry, Yarmouk University, Irbid, Jordan.

Research Experience

- 2025–Present:** Assistant Professor, Department of Pharmacy, Al-Zaytoonah University of Jordan, Amman, Jordan.
▶ Project 1: Virtual Screening of Natural Product Compounds Targeting breast cancer proteins for Cancer Therapeutics.
▶ Project 2: Targeting Aldehyde Dehydrogenase: A Virtual Screening Approach Using Natural Product Databases.
▶ Project 3: Molecular Docking of Urease Inhibitors: A Step Towards New Treatments for Gastric Ulcers
- 2022–2024:** Assistant Professor, Department of Pharmacy, Al-Zaytoonah University of Jordan, Amman, Jordan.
▶ Project 1: Computational studies on SARS-CoV-2 proteins.
▶ Project 2: Computational studies on peptide inhibitor of islet amyloid polypeptide aggregation associated with type II diabetes.
- 2021–2022:** Assistant Professor, Department of Chemistry, The University of Jordan, Amman, Jordan.
▶ Project: Computational studies on wild-type and top 4 mutant forms of p53 protein in human breast cancer.
- 2020–2021:** Assistant Professor, Department of Chemistry, The University of Jordan, Amman, Jordan.
▶ Project 1: Dynamical patterns of full-length human p53 protein: Computational study.

- ▶ Project 2: Virtual screening of in-house ligand library for potential anti-corona and anti-inflammatory drugs.

2009–2010: Postdoctoral Fellow, Department of Biochemistry and Molecular Biology, The University of Georgia, Athens, GA, USA

- ▶ Project: Structure and function of lung cancer related protein kinases.
Supervisor: Dr. Natarajan Kannan.

2006–2008: Research Assistant (PhD level), Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA

- ▶ Project 1: Ion permeation through membrane channels
Supervisors: Prof. Douglas J. Henderson and David D. Busath.
- ▶ Project 2: The radial distribution functions of highly asymmetric hard-sphere mixtures.
Supervisors: Prof. Douglas J. Henderson and David D. Busath.
- ▶ Project 3: The effect of dielectric polarization of the electrode on anomalous temperature effects in the electrical double layer using Monte Carlo simulation.
Supervisor: Prof. Douglas J. Henderson.
- ▶ Project 4: Monte Carlo simulation of the double layer at an electrode including the effect of a dielectric boundary.
Supervisor: Prof. Douglas J. Henderson.

1999–2001: Graduate Research Assistant (MS level), Department of Chemistry, Yarmouk University, Irbid, Jordan

- ▶ Project: The role of cyclodextrin cavity size on the normal and twisted intramolecular charge transfer (TICT) fluorescence of *N,N*-disubstituted *p*-cyanoanilines in aqueous solutions.
Supervisor: Prof. Khader Al-Hassan.

Peer-Reviewed Publications

- (1) **Mustafa, Morad;** Alwahsh, Mohammad; Hamadneh, Lama; Hasan, Aya; Abu-Irmaileh, Bashaer. *Integrated virtual and experimental screening of natural products as potential anticancer agents against breast cancer.* *Bioorganic Chemistry.* 2025; 166:109165. <https://doi.org/10.1016/j.bioorg.2025.109165>
- (2) Taher, Deeb; Saleh, Sundus; Habashneh, Almeqdad Y.; Hourani, Wafa; **Mustafa, Morad;** Helal, Wissam; Al-Noaimi, Mousa; Obeidat, Safwan M.; Kloda, Matous; Alhindi, Tareq; Kailani, Mohammed H.; Ghazzy, Asma. *Synthesis and anticancer activity of bis(β -ketoiminato) palladium(II) complexes of 3-[(chloro-substituted phenyl)amino]-1-phenyl-2-buten-1-one.* *Journal of Molecular Structure.* 2025; 1340:142542. <https://doi.org/10.1016/j.molstruc.2025.142542>
- (3) Taher, Deeb; Al-Said, Naim.H.; Albanna, Mohammad; Kloda, Matous; **Mustafa, Morad;** Helal, Wissam; Assaf, Khaleel I.; Hourani, Wafa; Kotob, Wael-Rémy; Saleh, Sundus; Makahleh, Ahmad; Rabba'a, Manar Mohammad. *Biological activity evaluation and molecular docking studies of newly synthesized β -ketoiminato-based palladium complexes.* *Inorganica Chimica Acta.* 2025; 583:122711. <https://doi.org/10.1016/j.ica.2025.122711>
- (4) Al Adem, Kenana; Ferreira, Juliana C.; Fadl, Samar; **Mustafa, Morad;** and Rabeh, Wael M. Key Allosteric and Active Site Residues of SARS-CoV-2 3CLpro Are Promising Drug Targets. *Biochemical Journal.* 2023; 480(11):791–813. <https://doi.org/10.1042/BCJ20230027>
- (5) Salman, Haya Ayyal; Yaakop, Amira Suriaty; Aladaileh, Saleem; **Mustafa, Morad;**

- Gharaibeh, Mohammed; Kahar, Ummirul Mukminin. Inhibitory effects of *Ephedra alte* on IL-10, IL-6, hybrid TLR4, TNF- α , IL-1 β , and extracted TLR4 receptors: in silico molecular docking. *Heliyon*. 2023; 9(1):e12730. <https://doi.org/10.1016/j.heliyon.2022.e12730>
- (6) Jamhour, Rasheed M. A. Q.; Al-Nadaf, Afaf H.; Wedian, Fadel; Al-Mazaideh, Ghassab M.; **Mustafa, Morad**; Huneif, Mohammed Aayed; Mahmoud, Sabry Younis; Farrag, Eman Saleh; Al-Rimawi, Fuad; Salman, Haya Ayyal; Alqudah, Ali Abdallah; Alakhras, Fadi. Phytochemicals as a potential inhibitor of COVID-19: An in silico perspective. *Russian Journal of Physical Chemistry A*. 2022; 96:1589–1597. <https://doi.org/10.1134/S0036024422070251>
- (7) **Mustafa, Morad**; Gharaibeh, Mohammad. Most Probable Druggable Pockets in Mutant p53-Arg175His Clusters Extracted from Gaussian Accelerated Molecular Dynamics Simulations. *Protein Journal*. 2022; 41:27–43. <https://doi.org/10.1007/s10930-022-10041-0>
- (8) **Mustafa, Morad**; Wedian, Fadel; Aldal'in, Hammad K.; Al-Mazaideh, Ghassab M.; Mahmoud, Sabry Younis; Farrag, Eman Saleh; Gharaibeh, Mohammed; Hijawi, Thameen; Al-Rimawi, Fuad; Abbadi, Jihad; Shalayel, Mohammed Helmy Faris; Siddique, Nadeem A.; Salman, Haya Ayyal; Huneif, Mohammed Aayed. The efficiency of some active ingredients of *Arum Palaestina* as inhibitors to 3CL^{pro} and Nsp15 proteins. *Acta Poloniae Pharmaceutica*. 2021;78(5):657–665.
- (9) **Mustafa, Morad**; Mirza, Amar; Kannan, Natarajan. Conformational regulation of the EGFR kinase core by the juxtamembrane and C-terminal tail: a molecular dynamics study. *Proteins*. 2011;79(1):99–114. <https://doi.org/10.1002/prot.22862>
- (10) Mirza, Amar; **Mustafa, Morad**; Talevich, Eric; Kannan, Natarajan. Co-conserved features associated with cis regulation of ErbB tyrosine kinases. *PLoS One*. 2010;5(12):e14310. <https://doi.org/10.1371/journal.pone.0014310>
- (11) **Mustafa, Morad**; Henderson, Douglas J.; Busath, David D. Free-energy profiles for ions in the influenza M₂-TMD channel. *Proteins*. 2009;76(4):794–807. <https://doi.org/10.1002/prot.22376>
- (12) **Mustafa, Morad**; Henderson, Douglas J.; Busath, David D. Computational studies of gramicidin permeation: an entryway sulfonate enhances cation occupancy at entry sites. *Biochimica et Biophysica Acta – Biomembranes*. 2009;1788(6):1404–1412. <https://doi.org/10.1016/j.bbamem.2009.03.021>
- (13) **Mustafa, Morad**; Busath, David D. The gramicidin channel ion permeation free-energy profile: direct and indirect effects of CHARMM force field improvements. *Interdisciplinary Sciences: Computational Life Sciences*. 2009;1(2):113–127. <https://doi.org/10.1007/s12539-009-0025-3>
- (14) Santos, Andrés; Yuste, Santos B.; López de Haro, Mariano; **Alawneh, Morad**; Henderson, Douglas. Contact values for disparate-size hard-sphere mixtures. *Molecular Physics*. 2009;107(7):685–691. <https://doi.org/10.1080/00268970902852665>
- (15) **Alawneh, Morad**; Henderson, Douglas; Outhwaite, Christopher W.; Bhuiyan, Lutful Bari. The effect of dielectric polarization of the electrode on anomalous temperature effects in the electrical double layer. *Molecular Simulation*. 2008;34(5):501–507. <https://doi.org/10.1080/08927020701654635>
- (16) **Alawneh, Morad**; Henderson, Douglas J. Molecular dynamics results for the radial distribution functions of highly asymmetric hard sphere mixtures. *Molecular Physics*. 2008;106(5):607–614. <https://doi.org/10.1080/00268970802116906>
- (17) Bhuiyan, Lutful Bari; Outhwaite, Christopher W.; Henderson, Douglas; **Alawneh, Morad**. A further Monte Carlo and modified poisson-boltzmann analysis of two recent results in the electric double layer theory. *Bangladesh Journal of Physics*. 2007;4:93–102.
- (18) Henderson, Douglas; **Alawneh, Morad**; Saavedra-Barrera, Rafael; Lozada-Cassou,

- Marcelo. Application of a recently proposed test to the hypernetted chain approximation for the electric double layer. *Condensed Matter Physics*. 2007;10(3(51)):323–330.
- (19) Bhuiyan, Lutful Bari; Outhwaite, Christopher W.; Henderson, Douglas; **Alawneh, Morad**. A modified poisson-boltzmann theory and Monte Carlo simulation study of surface polarization effects in the planar diffuse double layer. *Molecular Physics*. 2007;105(10):1395–1402. <https://doi.org/10.1080/00268970701355795>
- (20) **Alawneh, Morad**; Henderson, Douglas. Monte Carlo simulation of the double layer at an electrode including the effect of a dielectric boundary. *Molecular Simulation*. 2007;33(6):541–547. <https://doi.org/10.1080/08927020601054068>

Non-Refereed Publications

- (1) **Mustafa, Morad**. Ion permeation through membrane channels: molecular dynamics simulations studies. *Brigham Young University Dissertation*. Advisers: Prof Douglas J. Henderson and Prof David D. Busath.
- (2) **Mustafa, Morad**. The role of cyclodextrin cavity size on the normal and twisted intramolecular charge transfer (TICT) fluorescence of N,N-disubstituted p-cyanoanilines in aqueous solutions. *Yarmouk University Thesis*. Adviser: Prof Khader Al-Hassan

Refereed Articles

- (1) Ullah, Anwar and Ullah, Kifayat. Inhibition of SARS-CoV-2 3CL M^{pro} by natural and synthetic inhibitors: potential implication for vaccine production against COVID-19. *Frontiers in Molecular Biosciences*. 2021;8:640819.

Conferences, Symposiums, and Workshops

- (1) **Mustafa, Morad**; Mirza, Amar; Kannan, Natarajan. The structural impact of cancer mutations in EGFR using molecular dynamics simulations. Georgia Cancer Research Symposium. Nov 5–6, 2008; Athens, GA, USA [**Poster**].
- (2) **Mustafa, Morad**; Busath, David D. Molecular dynamics simulations of Na⁺ transport free-energy profile for gramicidin and two analogs. Joint Northwest and Rocky Mountain Regional Meeting of the American Chemical Society. Jun 15–18, 2008; Park City, UT, USA [Presentation].
- (3) Mustafa, Morad; Henderson, Douglas J.; Busath, David D. CMAP helps solve the gramicidin problem. Biophysical Society (52nd Annual Meeting). Feb 2–6, 2008. Long Beach, CA, USA [**Poster**].
- (4) **Mustafa, Morad**; Henderson, Douglas J.; Busath, David D. A comparative study of force fields for tryptophan with experiment using MD simulations. Telluride Science Research Center (Ion Channel Biophysics). Jul 30–Aug 3, 2007. Telluride, CO, USA [**Presentation**].
- (5) **Mustafa, Morad**; Henderson, Douglas J.; Busath, David D. Studying the influenza M₂ channel occupancy by other ions using MD simulations. Telluride Science Research Center (Ion Channel Biophysics). Jul 30–Aug 3, 2007. Telluride, CO, USA [Presentation].
- (6) **Mustafa, Morad**; Henderson, Douglas J.; Busath, David D. MD simulations of influenza M₂ using different cation sizes in a lipid bilayer. Biophysical Society (51st Annual Meeting). Mar 3–7, 2007. Baltimore, MD, USA [**Presentation**].
- (7) **Mustafa, Morad**; Henderson, Douglas J.; Busath, David D. MD simulations of gramicidin A and taurine gramicidin A in a lipid bilayer. Biophysical Society (51st Annual Meeting). Mar 3–7, 2007. Baltimore, MD, USA [**Poster**].

Research Grants & Funding

- None

Teaching Record

Department of Pharmacy, Al-Zaytoonah University of Jordan, Amman, Jordan.

- Undergraduate Courses
 - ▶ 0420820: General Chemistry for Pharmacy
 - ▶ 0420819: General Chemistry for Nursing
 - ▶ 0201143: General Chemistry for Engineering
 - ▶ 0201111: Physical Pharmacy
 - ▶ 0420821: General Chemistry Laboratory
 - ▶ 0201144: General Chemistry Laboratory for Engineering

Department of Chemistry, The University of Jordan, Amman, Jordan.

- Undergraduate Courses
 - ▶ Chem 101: General Chemistry 1
 - ▶ Chem 102: General Chemistry 2
 - ▶ Chem 109: General Chemistry Laboratory

Assistant Professor: Department of Chemistry, King Khalid University, Abha, Saudi Arabia.

- Undergraduate Courses
 - ▶ Chem 101: General Chemistry 1
 - ▶ Chem 107: General Chemistry for Engineers
 - ▶ Chem 231: Physical Chemistry for Chemical Engineering;
 - ▶ Chem 336: Kinetics and Reaction Mechanisms
 - ▶ Chem 436: Quantum Chemistry
 - ▶ Chem 470: Graduation Research
- Graduate Courses
 - ▶ Chem 531: Advanced Physical Chemistry
 - ▶ Chem 532: Quantum Chemistry and Applications

Graduate Teaching Assistant: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA

- Undergraduate Courses
 - ▶ Chem 103: Introductory Chemistry Laboratory
 - ▶ Chem 106: General College Chemistry
 - ▶ Chem 107: General College Chemistry Laboratory
 - ▶ Chem 213L: Introductory Inorganic Laboratory
 - ▶ Chem 227: Introductory Analytical Chemistry
 - ▶ Chem 227L: Introductory Analytical Chemistry Laboratory
 - ▶ Chem 461: Physical Chemistry
 - ▶ Chem 462: Physical Chemistry

Graduate Teaching Assistant: Department of Chemistry, Yarmouk University, Irbid, Jordan

- Undergraduate Courses
 - ▶ Chem 105: General Chemistry Laboratory I

- ▶ Chem 106: General Chemistry Laboratory II
- ▶ Chem 107: General Chemistry Laboratory
- ▶ Chem 213: Organic Chemistry Laboratory I
- ▶ Chem 232: Analytical Chemistry Laboratory

Membership of Committees

- Department of Pharmacy, Al-Zaytoonah University of Jordan, Jordan
 - ▶ Committee of Quality Assurance, 2023–present.
 - ▶ Committee of Computing and E-Learning, 2022–2023.
- Department of Chemistry, King Khalid University, Saudi Arabia
 - ▶ Unit of Strategic Planning, 2017–2018.
 - ▶ Committee of Strategic Planning, 2016–2017.
 - ▶ Committee of Website Development for College of Science, 2015–2017.
 - ▶ Committee of Academic Planning and Curriculum, 2014–2019.
 - ▶ Committee of Academic Schedules, 2011–2015.
 - ▶ Committee of Academic Advising, 2011–2015.

Professional and Scientific Meetings

- Participation in Scientific meetings
 - ▶ 9th International Pharmaceutical Conference, Department of Pharmacy, Al-Zaytoonah University of Jordan, Amman, Jordan, 16–17 October 2024.
- Scientific Meetings Organized
 - ▶ 5th International Chemistry Conference, Department of Chemistry, King Khalid University, Abha, Saudi Arabia, 26–29 April 2014.

Honors and Awards

- 2008: Travel Award (Biophysical Society in Long Beach, CA, USA).
- 2007: Travel Award (Biophysical Society in Baltimore, MD, USA).
- 2006: Outstanding Teaching Assistant Award (Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA).

Fellowships and Scholarships

- 2006–2008: Roland K. Robbins Graduate Research Fellowship (Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA).
- 2003–2008: Chemistry and Biochemistry Scholarship (Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, USA).

Professional Levels and Skills

Language Levels:

- ▶ Native Arabic speaker and writer
- ▶ Advanced Level (High Proficiency) in written and spoken English

Computer Skills:

- ▶ Operating Systems: Linux and Windows
- ▶ Office Suite: LibreOffice and Microsoft Office
- ▶ Programming Languages: Python and R
- ▶ Software Packages: LaTeX and Inkscape
- ▶ Web Content Management System: WordPress.

Computational Biophysical Chemistry Skills:

- ▶ Quantum Chemistry: Gaussian
- ▶ Molecular Dynamics: AMBER
- ▶ Computer-Aided Drug Design: Autodock Vina
- ▶ Molecular Visualization and Analysis: ChimeraX and LigPlot⁺.

Licenses and Certifications

- 2025: Certificate of Utilizing and Managing the E-Learning and Examination System. Accreditation and Quality Assurance Office, Al-Zaytoonah University of Jordan, Jordan.
- 2025: Certificate of Quality Assessor for Higher Education Institutions. Accreditation and Quality Assurance Commission for Higher Education Institutions, Jordan.
- 2022: License to Practice Academic Work OR Academic Work Permit. Ministry of Higher Education & Scientific Research, Jordan.
Academic Work at Universities and Community Colleges.
- 2022: Certificate of Workshop Completion. Use of Modern Teaching Methods and Educational Technology in Teaching and Learning for Practicing Academic Profession. The Center of Consultations and Training, The University of Jordan, Jordan.
- 2022: Certificate of Arabic Language Proficiency. The Jordan Academy of Arabic, Jordan.
- 2019: Certificate of Appreciation: Academic Planning and Curriculum Development. Department of Chemistry, King Khalid University, Saudi Arabia.
- 2017: Certificate of Appreciation: Development of a Strategic Plan. College of Science, King Khalid University, Saudi Arabia.
- 2013: Certificate of Appreciation: Academic Development and Quality. College of Science, King Khalid University, Saudi Arabia.

Supervision of Graduate Research

- Department of Pharmacy, Al-Zaytoonah University of Jordan, Jordan
 - ▶ None

Academic Program Development Record

- ▶ In collaboration with faculty members, I have developed several new academic courses for the new Bachelor of Science Program in Chemistry, Department of Chemistry, King Khalid University, Abha, Saudi Arabia.

Year 1

- ▶ University Chemistry
- ▶ University Chemistry Laboratory

Year 2

- ▶ Applied Calculus I
- ▶ Applied Calculus II
- ▶ Introductory Chemistry
- ▶ Introductory Chemistry Laboratory
- ▶ Inorganic Chemistry I
- ▶ Organic Chemistry I
- ▶ Organic Chemistry II
- ▶ Organic Chemistry Laboratory I

Year 3

- ▶ Applied Differential Equations
- ▶ Applied Electromagnetism
- ▶ Applied Electromagnetism Laboratory
- ▶ Inorganic Chemistry II
- ▶ Inorganic Chemistry Laboratory I
- ▶ Physical Chemistry I
- ▶ Physical Chemistry II
- ▶ Physical Chemistry Laboratory
- ▶ Interdisciplinary Chemistry I
- ▶ Interdisciplinary Chemistry II

Year 4

- ▶ Applied Statistics
- ▶ Organic Chemistry Laboratory II
- ▶ Inorganic Chemistry Laboratory II
- ▶ Organometallic Chemistry